Band Gap Tuning of Alumina by Surface Adsorption of p-group elements: A DFT Study

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We present a density functional theory study of the adsorption reactions of p-group atoms on the (0001) surface of the α-Al2O3. In this work, we work on α-Al2O3 (Corundum) monolayer and we found that the band gap 4.58 eV has been reduced compare to bulk structure 6.24 eV[1], which is tunable from insulator to semiconducting nature by adsorbing different solid and gas adatoms by using first-principles calculations. The effect of adsorption of p-group atoms such as metal atoms- B, C and gas atoms - N,O,F owing physisorption and chemisorptions process on the alumina (Al2O3) surface which have been systematically concluded by adsorption properties using density functional theory (DFT). Due to the hybridization of adsorbate selected elements, they help to tune the electronic properties along to the n-type and p-type direction, which light up the new way to develop cheap and possible device.[2,3] Presented adsorption process is also very clearly defined by adsorption energy, electronic band structure, projected density of state (PDOS), and electron localised function (ELF). We thus light up the way to producing a tuneable alumina band gap by adsorbing adatoms, which may play an important role in the utilisation of alumina in future alumina -based electronic nano-devices.

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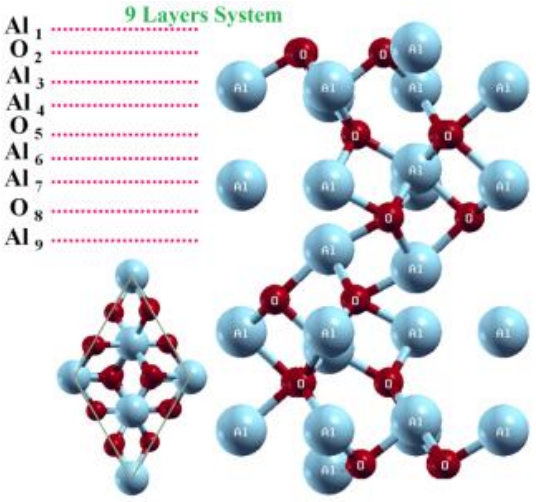

Figure: Top view (left side) and side view (right side) of our model of the α-Al2O3 (0001) surface. The relaxed structure is shown. The side view shows on the right the nine stoichiometric layers and on the left the layer labelling used. The colour code is red (oxygen) and blue (aluminium).